

Repulsively bound atom pairs: Overview, Simulations and Links

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Abstract. We review the basic physics of repulsively bound atom pairs in an optical lattice, which were recently observed in the laboratory [1], including the theory and the experimental implementation. We also briefly discuss related many-body numerical simulations, in which time-dependent Density Matrix Renormalisation Group (DMRG) methods are used to model the many-body physics of a collection of interacting pairs, and give a comparison of the single-particle quasimomentum distribution measured in the experiment and results from these simulations. We then give a short discussion of how these repulsively bound pairs relate to bound states in some other physical systems.

Keywords: optical lattices, repulsively bound pairs, Bose-Hubbard model, time-dependent Density Matrix Renormalization Group

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Introduction

Stable bound states, in which the composite object has a lower energy than the separated constituents, give rise to much diversity and complexity in many physical systems. Well-known examples ranging from chemically bound atomic molecules to excitons in solid state physics rely on attractive interactions to give rise to bound objects. The converse, particles bound by a repulsive interaction, is impossible in free space because interaction energy can be freely converted to kinetic energy of the constituent atoms. However, by placing particles on a lattice, kinetic energy is restricted to fall within the Bloch bands, and repulsively interacting atoms cannot always move apart and convert their interaction energy to kinetic energy. Recently we have reported on the first clear observation of such states, in the form of repulsively bound pairs of atoms in an optical lattice [1].

The stability of these pairs relies on the weak coupling of atoms in optical lattices to dissipative processes, which would otherwise lead to rapid relaxation of the system to its ground state (as is typically seen, e.g., in the context of solid state lattices). In this article we give an overview of repulsively bound atom pairs, beginning with a discussion of a single pair, and proceeding with a discussion of the experimental implementation, and many-body numerical simulations used to analyse a system of many interacting pairs. We then comment on analogies between these composite objects and bound states found

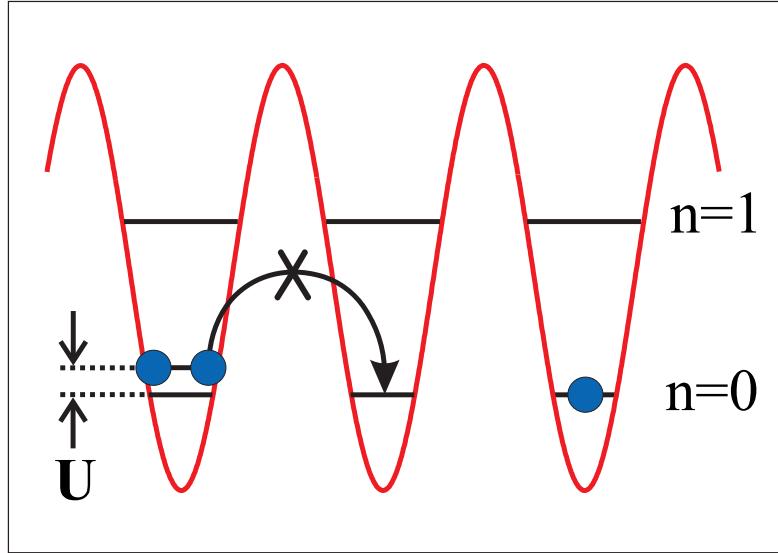


FIGURE 1. A state with two atoms located on the same site of an optical lattice has an energy offset $\approx U$ with respect to states where the atoms are separated. Breaking up of the pair is suppressed due to the lattice band structure and energy conservation, so that the pair remains bound as a composite object, which can tunnel through the lattice. In the figure, $n = 0$ denotes the lowest Bloch band and $n = 1$ the first excited band.

in other physical systems.

Repulsively bound atom pairs in an optical lattice

The existence of repulsively bound atom pairs is predicted by the Bose-Hubbard model [2], which describes well the dynamics of ultracold atoms loaded into the lowest band of a sufficiently deep optical lattice [3]. The corresponding Hamiltonian is

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1), \quad (1)$$

where \hat{b}_i (\hat{b}_i^\dagger) are destruction (creation) operators for the bosonic atoms at site i of the lattice, and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the corresponding number operator. J/\hbar denotes the nearest neighbor tunnelling rate, and U the on-site collisional energy shift. The relative value of U and J can be adjusted by varying the depth of the lattice V_0 .

In the limit of $U/J \rightarrow \infty$, the repulsively bound pair can be seen as an object where two atoms are located on the same lattice site. Due to the interaction between atoms, this state has an energy offset of U compared with states where atoms are present on different lattice sites. The stability of the pair can then be understood by energy conservation arguments: Two separated atoms moving in the lowest Bloch band of a lattice can have a maximum combined kinetic energy of $8J$ (in 1D). Thus, the atoms cannot separate and convert their interaction energy to kinetic energy (see Figure 1).

More generally, repulsively bound pairs arise from the eigenstates of the Bose-Hubbard model with two atoms present on the lattice. Denoting the primitive lattice vectors in each of the d dimensions by \mathbf{e}_i , we can write the position of the two atoms by $\mathbf{x} = \sum_{i=1}^d x_i \mathbf{e}_i$ and $\mathbf{y} = \sum_{i=1}^d y_i \mathbf{e}_i$, where x_i, y_i are integers, and we can write the two atom wave function in the form $\Psi(\mathbf{x}, \mathbf{y})$. The related Schrödinger equation from the Bose-Hubbard model then takes the form

$$[-J(\tilde{\Delta}_{\mathbf{x}}^0 + \tilde{\Delta}_{\mathbf{y}}^0) + U \delta_{\mathbf{x}, \mathbf{y}}] \Psi(\mathbf{x}, \mathbf{y}) = E \Psi(\mathbf{x}, \mathbf{y}), \quad (2)$$

where the operator

$$\tilde{\Delta}_{\mathbf{x}}^{\mathbf{K}} \Psi(\mathbf{x}) = \sum_{i=1}^d \cos(\mathbf{K} \mathbf{e}_i / 2) [\Psi(\mathbf{x} + \mathbf{e}_i) + \Psi(\mathbf{x} - \mathbf{e}_i) - 2\Psi(\mathbf{x})] \quad (3)$$

denotes the discrete lattice Laplacian on a cubic lattice. Writing the wavefunction in relative and centre of mass coordinates $\Psi(\mathbf{x}, \mathbf{y}) = \exp(i\mathbf{K}\mathbf{R}) \psi_{\mathbf{K}}(\mathbf{r})$, the Schrödinger equation can be reduced to a single particle problem in the relative coordinate

$$[-2J\tilde{\Delta}_{\mathbf{r}}^{\mathbf{K}} + E_{\mathbf{K}} + U \delta_{\mathbf{r}, 0}] \psi_{\mathbf{K}}(\mathbf{r}) = E \psi_{\mathbf{K}}(\mathbf{r}) \quad (4)$$

where $E_{\mathbf{K}} = 4J \sum_{i=1}^d [1 - \cos(\mathbf{K} \mathbf{e}_i / 2)]$ is the kinetic energy of the center of mass motion.

The short range interaction potential makes it possible to resum the perturbation expansion for the associated Lippman-Schwinger equation, and we obtain the scattering states

$$\psi_E(\mathbf{r}) = \exp(i\mathbf{K}\mathbf{r}) - 8\pi J f_E(\mathbf{K}) G_{\mathbf{K}}(E, \mathbf{r}) \quad (5)$$

with scattering amplitude

$$f_E(\mathbf{K}) = -\frac{1}{4\pi} \frac{U/(2J)}{1 - G_{\mathbf{K}}(E, 0)U} \quad (6)$$

with total energy $E = \varepsilon_{\mathbf{k}, \mathbf{K}} + E_{\mathbf{K}}$, and $\varepsilon_{\mathbf{k}, \mathbf{K}} = 4J \sum_{i=1}^d \cos(\mathbf{K} \mathbf{e}_i / 2) [1 - \cos(\mathbf{k} \mathbf{e}_i)]$. Furthermore, $G_{\mathbf{K}}(E, \mathbf{r})$ denotes the Greens function of the non-interacting problem, which in Fourier space takes the form $\tilde{G}_{\mathbf{K}}(E, \mathbf{k}) = 1/(E - \varepsilon_{\mathbf{k}, \mathbf{K}} - E_{\mathbf{K}} + i\eta)$. The scattering states $\psi_E(\mathbf{r})$ correspond to two free atoms moving on the lattice and undergoing scattering processes.

In addition, the pole in the scattering amplitude indicates the presence of an additional bound state for each value of \mathbf{K} , which corresponds to the repulsively bound pair. The energy E_{bs} of the bound states is determined by $1 = U G_{\mathbf{K}}(E_{\text{bs}}, 0)$ while the bound state wave function takes the form $\psi_{\mathbf{K}}^{\text{bs}}(\mathbf{r}) = c G_{\mathbf{K}}(E_{\text{bs}}, \mathbf{r})$ with c a normalization factor. Note that in one dimension such bound states exists for arbitrary repulsive interaction, but for a three-dimensional lattice such bound states, and therefore repulsively bound pairs, appear only for a repulsive interaction above a critical value $U > U_{\text{crit}} \approx 8J$ (for $K = 0$). These states have a square-integrable relative wavefunction $\psi_{\mathbf{K}}(\mathbf{r})$, as shown for two different values of U/J in Figure 2. For a deep lattice, i.e. $U/J \gg 1$, bound pairs essentially consist of two atoms occupying the same site, whereas for small U/J , the pair is delocalized over several lattice sites. A main feature of the repulsive pair wavefunction

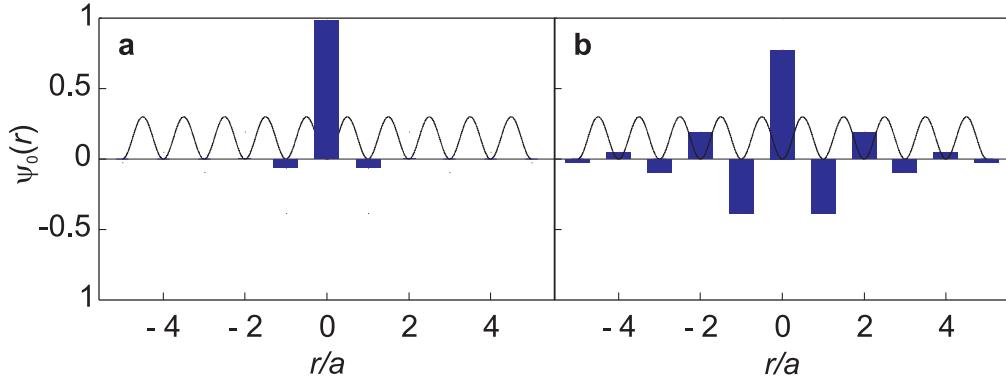


FIGURE 2. Relative wavefunctions $\psi_0(\mathbf{r})$ for repulsively bound pairs ($a_s = 100a_0$) in 1D with $K = 0$, for (a) $U/J = 30$ ($V_0 = 10E_r$) and (b) $U/J = 3$ ($V_0 = 3E_r$), where E_r is the recoil energy. ($E_r = 2\pi^2\hbar^2/m\lambda^2$, where m is the mass of the atoms and λ is the twice the lattice period, a .)

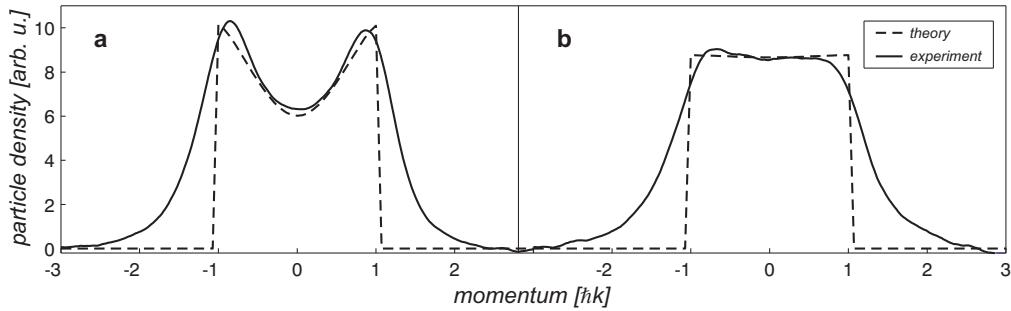


FIGURE 3. Single particle quasimomentum distributions for repulsively bound pairs in 1D from experiment and numerical simulations (see text) for (a) $V_0 = 5E_R$ and (b) $V_0 = 20E_R$. The density values have been scaled to facilitate comparison between experimental and theoretical results. These results agree well, up to experimental artifacts related to repulsion between atoms during expansion (before imaging) and also relatively long imaging times (many photons are scattered from each atom, which performs a random walk). This leads to smearing out of the sharp structure at the edge of the Brillouin zone.

is its oscillating character: the wavefunction amplitude alternates sign from one site to the next. In quasimomentum space this corresponds to a wavefunction which is peaked at the edges of the first Brillouin zone, as is shown in Figure 3.

When many repulsively bound pairs exist, they will interact with one another as described by the Bose-Hubbard model. This many-body behaviour can be computed numerically as described below.

Experimental realization of repulsively bound atom pairs

We experimentally create repulsively bound atom pairs from a sample of ultracold ^{87}Rb atoms in a cubic 3D optical lattice. About 2×10^4 atom pairs are initially prepared in a deep lattice of $35E_r$ depth, with each site of the lattice either doubly-occupied or unoccupied. By adiabatically ramping down the lattice depth afterwards the initially

localized pair wavefunctions become delocalized (see Fig. 2). The initial preparation is carried out in several steps as described in the following. In the beginning, a Bose Einstein condensate of ^{87}Rb atoms is carefully loaded into the vibrational ground state of the optical lattice, such that many lattice sites are occupied with two atoms. Besides the doubly occupied sites, there are also sites which are occupied by single atoms or more than two atoms. In order to remove atoms from these sites we use a purification scheme which involves the use of a Feshbach resonance and a combined pulse of laser and radio-frequency (rf) radiation [4]. The laser and rf pulse resonantly blows atoms out of the lattice, whereas the Feshbach resonance serves to protect (shelve) the pairs temporarily from this pulse by converting pairs into Feshbach molecules and then back into atoms. Besides lifetime measurements, we have been able to experimentally map out the single particle momentum distribution (see Fig. 3) and to measure their binding energy. The properties and the dynamics of the pairs can be controlled by tuning the atom-atom interaction with the help of a Feshbach resonance at 1007G and by controlling the depth of the optical lattice and particle density. Consistent with our theoretical analysis, the repulsively bound pairs exhibit long lifetimes of hundreds of milliseconds, even under collisions with one another.

Many-Body simulations

Many-body numerical simulations for a gas of repulsively bound pairs are performed using time-dependent DMRG methods [5]. These methods allow for ground state calculation and time-dependent calculation of the dynamics of atoms for a variety of 1D situations, including many lattice and spin models. The basic algorithm provides near-exact integration of a many-body Schrödinger equation, with the Hilbert space being adaptively decimated. This works provided that the state of the system is always able to be efficiently represented as a matrix product state [6]. As a result, it is possible to compare the dynamics of a gas of interacting repulsively bound pairs in a 1D lattice with experimental data. For example, we can simulate a 1D Bose-Hubbard model with time dependent parameters, beginning with an initial state corresponding to a distribution of atoms situated in doubly occupied lattice sites. We compute the corresponding dynamics as the lattice depth is decreased by decreasing U and increasing J . These many-body simulations account for interactions between bound pairs, and let us compute final momentum distributions that agree well with the experimental results. We can also use these simulations to model lattice modulation spectroscopy of atoms in optical lattices. In figure 3 we show a comparison of quasimomentum distributions from the experiment and from many-body simulations.

Analogy to Other Bound States

Although no stable repulsively bound pairs have previously been observed, they have an interesting relationship to many bound states in other physical systems. For example, resonance behaviour based on similar pairing of Fermions of different spin

in the Hubbard model was first discussed by Yang [7], and plays an important role in SO(5) theories of superconductivity [8]. There are several examples of many-body bound states that can occur for repulsive as well as attractive interactions, such as the resonances discussed in the context of the Hubbard model by Demler et al. [9]. Such resonance behaviour is common in many-body physics, although states of this type are normally very short-lived. Optical lattice experiments will now provide an opportunity to prepare and investigate stable versions of such states, which until now have only appeared virtually as part of complex processes.

The stability and many-body physics of repulsively bound pairs is perhaps most closely associated with that of excitons, which are bound pairs of a particle in the conduction band and a hole in the valence band of a periodic system [10]. These bind to form a composite boson, a gas of which can, in principle, Bose-condense. Excitons are excited states of the many-body system, but are bound by an attractive interaction between the particle and hole that form the pair. They are also discussed in the specific context of fermionic systems. However, a single exciton on a lattice could have a description very similar to that of a single repulsively bound pair, and could be realised and probed in optical lattices experiments [11].

Repulsively bound atom pairs in an optical lattice are also reminiscent of photons being trapped by impurities in photonic crystals [12], which consist of transparent material with periodically changing index of refraction. An impurity in that crystal in form of a local region of index of refraction can then give rise to a localized field eigenmode. In an analogous sense, each atom in a repulsively bound pair could be as an impurity that “traps” the other atom.

An analogy can also be drawn between repulsively bound atom pairs and gap solitons, especially as found in atomic gases [13, 14, 15, 16]. Solitons are normally a non-linear wave phenomenon, and in this sense have a very different behaviour to repulsively bound pairs, which exhibit properties characteristic of many-body quantum systems. However, there has been increasing recent interest in discussing the limit of solitons in atomic systems where very few atoms are present, giving rise to objects that are often referred to as quantum solitons [17]. These are N-body bound states in 1D, and thus a 2-atom bright quantum soliton is a bound state of two atoms moving in 1D. In this sense, the solution for a single repulsively bound pair in 1D is related to a single quantum soliton on a lattice.

Conclusion

In summary, a metastable bound state that arises from repulsion between the constituents and the lattice band structure has been demonstrated in the laboratory. This state exemplifies in a new way the strong correspondence between the optical lattice physics of ultracold atoms and the Hubbard model, a connection which has particular importance for applications of these cold atom systems to more general simulation of condensed matter models, to quantum computing. The existence of such metastable bound objects will be ubiquitous in cold atoms lattice physics, giving rise to new potential composite objects also in Fermions or in systems with mixed Bose-Fermi statistics.

These states could also be formed with more than two particles, or as bound states of existing composite particles. Repulsively bound pairs have no counterpart in condensed matter physics due to the strong inelastic decay channels observed in solid state lattices, and could be a building block of yet unstudied quantum many body states or phases.

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